Effective temperature and compactivity of a lattice-gas under gravity

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The notion of longitudinal effective temperature and its relation with the Edwards compactivity are investigated in an abstract lattice gas model of granular material compacting under gravity and weak thermal vibration.

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A distinctive feature of mean-field glassy dynamics is a peculiar violation of fluctuation-dissipation relations which leads to the definition of a time-scale dependent "effective temperature" [1,2], and the possibility of constructing a non-equilibrium thermodynamics of glasses and dense granular media [3,4]. Effective temperature also appears in athermal systems, where the high packing density regime is attained by compression or by using a confining potential. A particularly interesting situation, which is relevant to the study of granular materials, occurs when the confining force is gravity. In this case a non stationary inhomogeneous density profile generally arises and the notion of effective temperature may be then not well defined unless suitable conditions are verified. In this note we explore the possibility of defining a global effective temperature in an abstract model of granular material under gravity and weak thermal vibration, and its relation with the Edwards compactivity.

The model consists of a gas of N particles on a body centred cubic (bcc) lattice where there can be at most one particle per site. There is no cohesion energy among particles and the Hamiltonian is

$$\mathcal{H}_0 = mg \sum_{i=1}^{N} h_i \, , \tag{1}$$

where g is the gravity constant, h_i is the height of the particle i, and m its mass. At each time step a particle can move with probability p to a neighboring empty site if the particle has less than ν nearest neighbors before and after it has moved [5]. Here $p = \min[1, x^{-\Delta h}]$ where $\Delta h = \pm 1$ is the vertical displacement in the attempted elementary move [6], and $x = \exp(-mg/k_{\rm B}T)$. We set $mg/k_{\rm B} = 1$ and $\nu = 4$ throughout. At high enough packing density, dynamical models of this kind possess an extensive entropy of blocked states (defined as configurations in which any particle is unable to move) whose derivative is the so-called Edwards compactivity. For this reason such models exhibit a slow compaction dynamics reminiscent of dense granular matter [7,8]. It was found in particular that during compaction a generalized fluctuation-dissipation relationship is obeyed [9], giving a first evidence of an effective temperature in this regime. In Ref. [9] the drift contribution to the longitudinal mean-square displacement was ignored [10], leading to claim that "all measures of vertical correlation and response lead to the impossibility of defining effective temperature" and that "the vertical drift due to compaction leads to contradictory results" [11]. Here we show that there are no such contradictory results: in the slow compaction regime the drift brings no qualitative change in the generalized fluctuation-dissipation relation found in Ref. [9], and its effect is substantially negligible at high packing density.

The fluctuation-dissipation properties can be characterized by applying a random perturbation to the system at times $t \geq t_{\rm w}$:

$$\mathcal{H}_\epsilon = \mathcal{H}_0 + \epsilon \, \Theta(t - t_{\rm w}) \sum_{i=1}^{N} f_i \, h_i \; , \tag{2}$$

where $f_i = \pm 1$ independently for each particle, ϵ is small enough to probe the linear response regime, and Θ is the step function. The integrated response function is then defined as:

$$\chi(t, t_{\rm w}) = \frac{1}{N} \sum_{i=1}^{N} \left\langle \overline{f_i \Delta h_i(t)} \right\rangle , \tag{3}$$

where $\Delta h_i(t)$ is the height difference between the perturbed and unperturbed i particle at time t. The angular brackets denote the average over the thermal noise while the overline denotes the average over the random force. The 'mean-square displacement' between two configurations at time $t_{\rm w}$ and $t > t_{\rm w}$ is:

$$B(t, t_{\rm w}) = \frac{1}{N} \sum_{i=1}^{N} \left\langle \Big[h_i(t) - h_i(t_{\rm w}) + \tilde{h}(t_{\rm w}) - \tilde{h}(t) \Big]^2 \right\rangle , \tag{4}$$

where the drift motion is taken into account by the average height:

$$\tilde{h}(t) = \frac{1}{N} \sum_{i=1}^{N} \langle h_i(t) \rangle \; . \tag{5}$$

Fig. 1 reports a parametric plot of mean-square displacement vs. response function at waiting time $t_{\rm w} = 2^{13}$: it clearly shows that the presence of a slow longitudinal drift does not prevent the existence of generalized

fluctuation-dissipation relation. In particular, no qualitative change occurs in the characteristic broken-line pattern when the drift term $\tilde{h}(t_\mathrm{w}) - \tilde{h}(t)$ in Eq. (4) is neglected, while appreciable quantitative deviations between the two sets of data (with and without the drift term) only appear when the measurement time is quite long. Similar results were also found in the so-called FILG model under gravity [12].

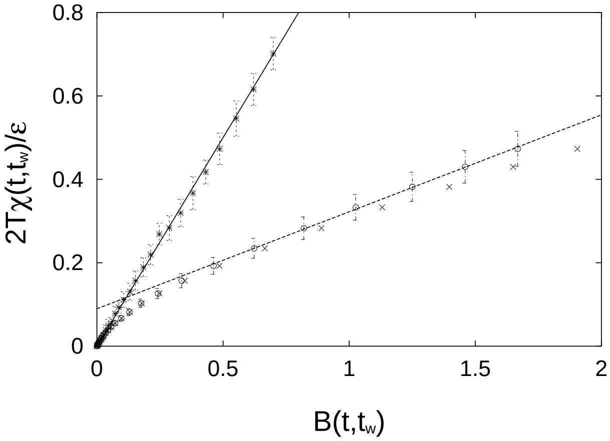

FIG. 1. Parametric plot of mean-square displacement $B(t, t_\mathrm{w})$ vs. response function $2T\chi(t, t_\mathrm{w})/\epsilon$, during compaction dynamics (circle symbols). The system is prepared in a random loose packed state with average density $\rho_\mathrm{rlp} \simeq 0.707$, and evolves under gravity and thermal vibration with $x = \exp(-1/T) = 0.2$. The perturbation is turned on at the waiting time $t_\mathrm{w} = 2^{13}$ and measurements are carried out for times t in the range $[t_\mathrm{w},\, t_\mathrm{w} + 10^5]$. The slope of the dashed line is 0.23 (to be compared with 0.20 obtained by neglecting the drift term ($\times$ symbols)). The solid line with slope one is the equilibrium fluctuation-dissipation theorem, which is recovered by removing kinetic constraints (star symbols).

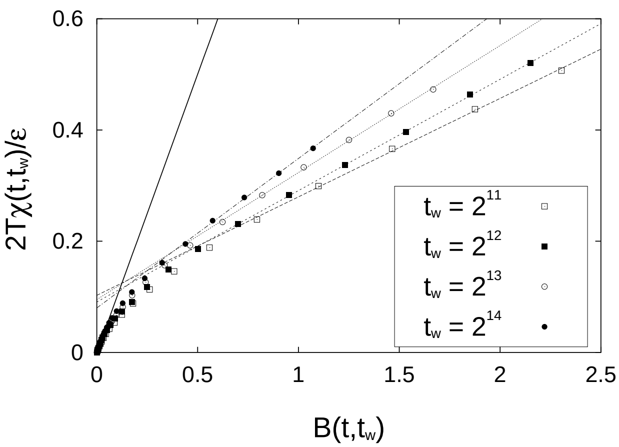

FIG. 2. Non-equilibrium fluctuation-dissipation relation in a compaction experiment as in FIG. 1, at different waiting times t_w. The slope of the straight lines is 0.18, 0.20, 0.23, and 0.27, for increasing waiting time.

The second result of the numerical compaction experiment is reported in Fig. 2: it shows that the generalized fluctuation-dissipation relation is obeyed at different waiting times. From the parametric plot of $\chi(t, t_\mathrm{w})$ vs. $B(t, t_\mathrm{w})$ one can define a time scale dependent effective temperature by means of the relation:

$$T_\mathrm{dyn}(t, t_\mathrm{w}) = \frac{\epsilon}{2} \frac{B(t, t_\mathrm{w})}{\chi(t, t_\mathrm{w})}\,, \qquad (6)$$

provided T_dyn is constant on that time scale, and where now it is understood a possible dependence of T_dyn on the density profile. Indeed, during compaction the system develops inhomogeneous density profiles [7,8], as it also happens after a sudden compression in zero gravity [13], and one may wonder about their influence on the effective temperature. In Ref. [8] the *stationary* density profile was interpreted as formed by two parts: a lower flat part at critical density $\rho_\mathrm{c} \simeq 0.84$, and an upper equilibrium part in which kinetic constraints play no role. Fig. 3 shows the temporal evolution of the density profile corresponding to the above compaction experiment: one observes that the upper part of the bulk density profile increases faster than the lower one (even when the former become denser than the latter), and that the bulk profile is far from being flat (see inset of Fig. 3). At late time the contribution of the top free interface is small for weak vibration, and - if sizeable - it would make higher the slope T/T_dyn, of the fluctuation-dissipation plot (i.e. smaller the effective temperature). While the contribution of particles at the bottom is negligible as they do not evolve at all.

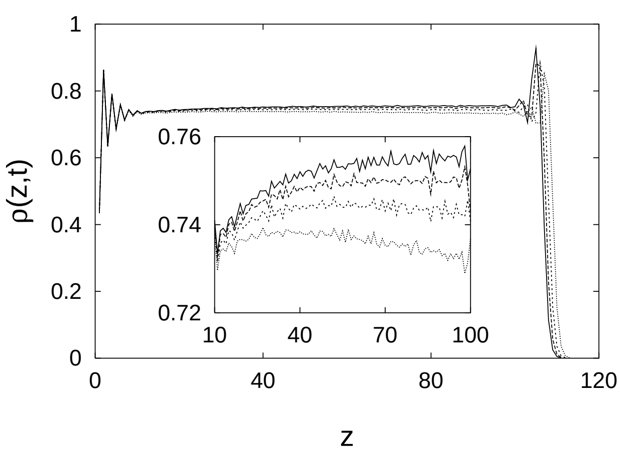

FIG. 3. Temporal evolution of the density profile during compaction dynamics ($x = 0.2$, and time $t = 2^{10+k}$ for $k = 1$ to 4). Inset: bulk density profile.

That the generalized fluctuation-dissipation relation is not affected *qualitatively* by an inhomogeneous density profile can be understood in terms of the mean-field dynamical model introduced in [13], and further generalized to nonzero gravity in [8]. In both cases the long-time relaxation of the local density factorizes:

$\rho_c - \rho(z,t) = f(z)\,g(t)$. Since the mean square displacement can be written as $B(z,t,t_w) = F(z)\,G(t,t_w)$ on long enough time interval $t - t_w$, the violation factor entails two independent contributions: a purely geometric factor and a purely dynamic one. The latter contribution is only responsible for the intrinsic violation of the fluctuation-dissipation relation. The notion of effective temperature therefore seems to be still reliable provided a geometric factor is taken into account (in this specific case the global geometric factor entering Eq. (6) would be $\mathcal{F} = \int f(z)\mathrm{d}z / \int F(z)\mathrm{d}z$). Notice that for a purely flat density profile there is no difference between 'horizontal' and 'vertical' observables, (and $\mathcal{F} = 1$).

The question that naturally arises is whether the longitudinal effective temperature can be interpreted in terms of the Edwards measure, which should now be obtained *by fixing the density profile of the experimental situation one wishes to reproduce* [14]. The numerical implementation of this strategy is however not straightforward. A more pragmatic approach consists in fixing a few feature of the profile (as suggested in this case by the expression of $\mathcal{F}$), such as average density, average slope and so on. This is quite similar in spirit to the construction of restricted Edwards measure which has been recently exploited in Ref. [15,16], and generally improves the comparison with numerical experiments.

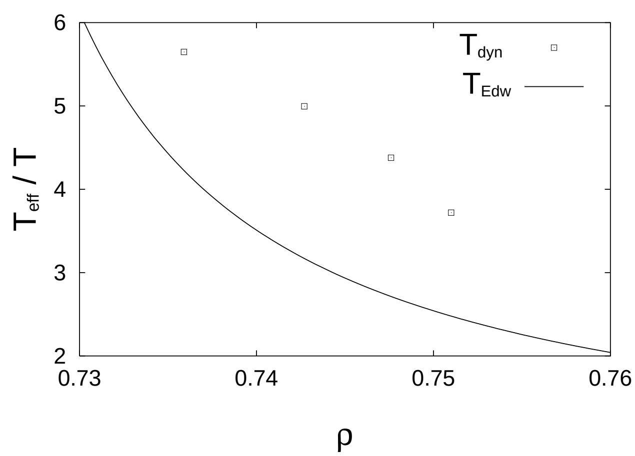

FIG. 4. Comparison between effective temperatures: $T_{\rm dyn}$ is measured during the compaction experiment from the fluctuation-dissipation relation at time t_w. $T_{\rm Edw}$ is approximated through the Edwards measure with a homogeneous density ρ such that the average bulk density profile at time t_w of the compaction experiment is $\rho_{\rm av}(t_w) = \rho$.

As a preliminary attempt to relate the effective temperature $T_{\rm dyn}$, to the inverse compactivity $T_{\rm Edw}$, we have computed the Edwards entropy $s_{\rm Edw}(\rho)$ to the lowest approximation, i.e. just by fixing a homogeneous density. In passing, the definition of blocked configuration in presence of gravity requires here some care: if one assumes a flat profile, it is not clear why blocked configurations should depend upon gravity, like in the definition adopted in Ref. [11]. We have therefore explicitly checked that there is no dependence upon gravity for the bcc lattice. This is not however the most general case: interestingly, we found that for the simple cubic lattice, the anisotropy due to gravity, (say along the direction 001), suppresses the first order character of the phase transition present in the Edwards measure at density below ≈ 0.7, [17]. We have then estimated $T_{\rm Edw}(\rho)$ from the relation:

$$T_{\rm Edw}\,\frac{\mathrm{d}s_{\rm Edw}}{\mathrm{d}\rho} = T\,\frac{\mathrm{d}s}{\mathrm{d}\rho}\,, \tag{7}$$

where $s(\rho) = -\rho\log\rho - (1-\rho)\log(1-\rho)$ is the equilibrium entropy [18]. The two effective temperatures, $T_{\rm Edw}$ and $T_{\rm dyn}$, are shown in Fig. 4 at several densities corresponding to the average bulk density profiles of the compaction experiment. It is clear that a ponderable comparison is possible only when other features of the density profile (e.g. the average slope) are fixed, but much work is needed to test this point.

In conclusion, we confirm the existence of a generalized fluctuation-dissipation relation in an abstract model of dense granular matter which exhibits non-stationary inhomogeneous density profiles. The occurrence of a longitudinal effective temperature in the slow compaction regime has been justified by a mean-field dynamical model and its relation with the Edwards compactivity has been discussed.

J.J. Arenzon, A. Barrat and S. Franz are acknowledged for discussions and comments.

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[14] This is indeed suggested by the functional nature of the nonzero gravity lattice gas entropy. For example, in the non-interacting case, Hamiltonian Eq. (1), the equilibrium entropy is

$$s[\rho] = -\sum_z \left\{ \rho(z) \log \rho(z) + [1-\rho(z)] \log [1-\rho(z)] \right\} .$$

From the minimization of the free energy one then gets

$$\frac{mgz}{T} = \frac{\delta s}{\delta \rho(z)} .$$

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[18] Notice that in the inhomogeneous case – when the entropy is a functional of the density profile, the functional version of Eq. (7) holds, and $T_{\rm Edw}$ will only depend on the density profile provided its thermodynamic interpretation holds true.